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Recent Livermore Excitation and Dielectronic Recombination Measurements for Laboratory and Astrophysical Spectral Modeling

P. Beiersdorfer^a, G. V. Brown^a, M.-F. Gu^b, C. L. Harris^c, S. M. Kahn^b, S.-H. Kim^d, P. A. Neill^c, D. W. Savin^b, A. J. Smith^e, S. B. Utter^a, and K. L. Wong^a

^a High-Temperature and Astrophysics Division,

Lawrence Livermore National Laboratory, Livermore, CA 94550, USA

^b Department of Physics, Columbia University, New York, NY 10027, USA

^c Department of Physics, University of Nevada, Reno, NV 89557, USA

^d Department of Physics, Pohang University of Science and Technology, Pohang, 790784,

^eDepartment of Physics, Morehouse College, Atlanta GA 30314, USA

Abstract

Using the EBIT facility in Livermore we produce definitive atomic data for input into spectral synthesis codes. Recent measurements of line excitation and dielectronic recombination of highly charged K-shell and L-shell ions are presented to illustrate this point.

I Introduction

X-ray spectroscopic measurements using the Livermore Electron Beam Ion Trap (EBIT) have been optimized over the past decade to provide definitive values of electron-impact excitation, ionization, and resonance excitation cross sections, as well as dielectronic resonance strengths. These measurements have covered a great number of excitation and recombination processes. Recent results have demonstrated several shortcomings of theoretical data. For example, the dielectronic recombination satellite emission involving spectator electrons with $n \geq 4$ contributing to the K β (3 \rightarrow 1) emission in heliumlike Ar¹⁶⁺ was shown to be considerably larger than expected from standard scaling procedures [1]. This EBIT result has now lead to a reassessment of line profile calculations of the heliumlike Ar^{16+} K β resonance line used for density diagnostics in laser fusion. Moreover, 30 years of calculations were shown to be unable to predict a reliable ratio for the singlet to triplet ratio of the $3d \rightarrow 2p$ line emission in neonlike Fe¹⁶⁺ [2]. The EBIT value for this ratio is in better agreement with theoretical data from 1967 [3] than with any calculation published since, despite the introduction of improved calculational techniques. The laboratory value markedly changed the amount of resonant scattering of the strong Fe¹⁶⁺ lines infered from solar corona observations. A third example is provided by measurements of the radiative power loss from highly charged krypton ions (Kr³⁰⁺ through Kr³⁴⁺) performed at the EBIT facility in Berlin [4]. The measured radiative power loss exceeds that calculated with the average-ion model used in fusion [5] by a factor of two and also exceeds that of more refined model calculations using a fully collisonal-radiative model [6]. The higher rate impacts the design of radiative divertors and the power balance in tokamaks.

As the examples above illustrate, EBIT measurements are needed not only to assess the accuracy of theoretical data, but are now urgently needed to provide definitive data in areas in which calculations fail to produce atomic data with the accuracy required for spectral modeling. In the following, we present recent work at the Livermore EBIT facility relevant to laboratory and astrophysical plasma modeling that further illustrate this need.

II Intensity Ratio of $3 \rightarrow 1$ Lines in Heliumlike Ions

Using high-resolution crystal spectrometers, we have carried out systematic measurements of the $3 \to 1$ line emission from heliumlike ions. We have found significant disagrement between the measured and calculated ratios of the $1s3p\ ^3P_1 \to 1s^2\ ^1S_0$ intercombination and the $1s3p\ ^1P_1 \to 1s^2\ ^1S_0$ resonance line in low and medium Z ions [7]. This disagreement is illustrated in Fig. 1(a). The figure plots the ratios measured just above threshold for electron-impact excitation where direct electron-impact excitation is the only line formation mechanism. Also shown are the results from two theoretical calculations. The first uses the distorted wave code from Zhang et al. [8], the second the HULLAC package [9]. While the cross sections calculated with each code agree with each other, the final results differ significantly from the measured ratios. The reason is that the 1s3p levels have radiative decay channels besides deexcitation to ground. Consequently, the calculated excitation cross sections must be multiplied by the appropriate radiative branching fractions. In the first case, the branching fractions calculated with the MCDF method were used; in the second case, fractions calculated by the HULLAC package were used. These two methods produce significantly different branching ratios, as illustrated in Fig. 1(b). These differences are

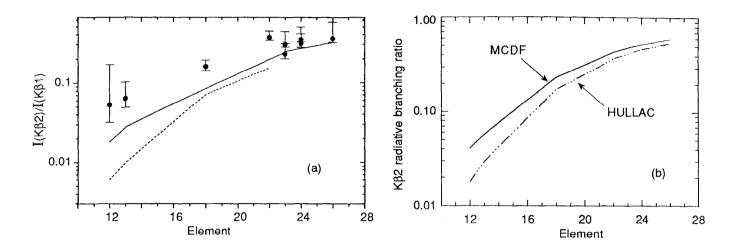


Figure 1: (a) Ratio of intercombination to resonance line in heliumlike $K\beta$ spectra. The solid line (dashed line) represents calculations with the distorted-wave code of Sampson and Zhang (HULLAC); (b) Radiative branching ratio of the heliumlike $K\beta$ line calculated with MCDF and HULLAC codes. (From [7].)

largest for the lower-Z heliumlike ions.

Uncertainties in the radiative rates alone, however, cannot explain all of the discrepancy between the calculated and observed line ratios. Calculations based on the relativistic configuration interaction method, which are deemed reliable to within about 1 %, have indicated that the actual branching fraction lies somewhere inbetween the two calculations shown in Fig. 1(b). Therefore, no further improvement of theory relative to experiment can be expected, even if very accurate branching fractions become available. Instead, part of the disagreement is likely to be due to inaccuracies in the distorted wave calculations.

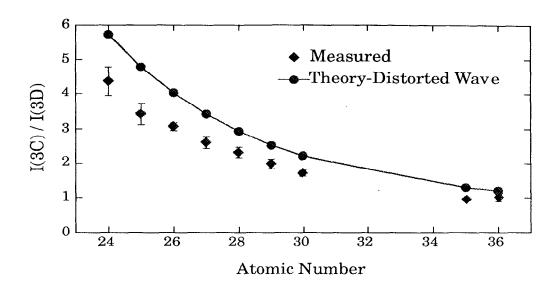


Figure 2: Ratio of intercombination and resonance line in neonlike ions. The solid line repesents results calculated in the distorted-wave approximation. (From [10].)

III Intensity Ratio of $3 \rightarrow 2$ Lines in Neonlike Ions

A detailed study of the line emission of neonlike Fe¹⁶⁺ has found significant disagrement between the measured and calculated ratios of the $2p^53d~^3D_1 \rightarrow 2p^6~^1S_0$ intercombination and the $2p^53d~^1P_1 \rightarrow 2p^6~^1S_0$ resonance line [2]. We have now completed a measurement of this line ratio as a function of Z and have uncovered a systematic disagreement for all ions studied [10]. The results are shown in Fig. 2.

Unlike the heliumlike $1s3p \ ^3P_1 \rightarrow 1s^2 \ ^1S_0$ lines the neonlike lines decay essentially 100% to ground. Errors in radiative rates should, therefore, not be the reason for the disagreement. The disagreement must instead be caused by inaccuracies in the distorted-wave calculations of the excitation cross sections. These measurements confirm the problems uncovered with

the Fe¹⁶⁺ ratio [2] mentioned in the introduction and show that they extend along the isoelectronic sequence.

IV Dielectronic Recombination Contributions to L-shell Lines

An area that has received essentially no theoretical or experimental attention is the contributions to L-shell emission lines from resonance excitation and high-n dielectronic satellites. We have made a systematic effort to measure all L-shell transitions in neonlike through lithiumlike iron, Fe¹⁶⁺ - Fe²³⁺. An inventory of these lines is given by Brown et al. [11]. An example of our measurements of the line formation processes producing a $3d \rightarrow 2p$ line in lithiumlike Fe²³⁺ is shown in Fig. 3. Our measurements clearly show the different contributions to the line: direct electron-impact excitation and resonance excitation above 1.2 keV, high-n satellites below. Resonance excitation has been calculated in the iron project [12]; agreement with our measurements is marginal. The energy grid of these calculations is coarse, so that resonances are easily missed. Those that are not missed are given additional weight, so that agreement with our measurements is in part fortuitous (cf. Gu et al. [13]). The status of calculations is worse for high-n satellites. As illustrated in Fig. 3, the high-n satellites contribute a considerable fraction of the total line emission. These satellites blend with the resonance lines and spectroscopically cannot be resolved, and thus must be included to properly model astrophysical or laboratory spectra. At present, calculations of the satellites below threshold have not been carried out for most L-shell lines. We will soon have completed our measurement of all of the relevant satellite and resonance contributions

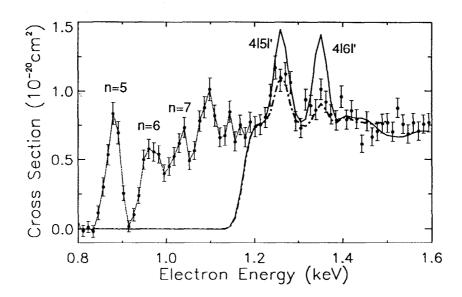


Figure 3: Excitation of the $3d_{5/2} \rightarrow 2p_{3/2}$ transition in lithiumlike Fe²³⁺. The solid line represents Iron Project calculations using the R-matrix method; the dashed line represents subsequent R-matrix calculations employing a much finer energy grid. (From [13].)

for strong Fe¹⁶⁺ – Fe²³⁺ lines making the need for calculations disappear.

V Conclusion

We have presented several recent results of our ongoing spectroscopic effort to provide atomic data for spectral modeling. We have illustrated several cases where measurements are more reliable and complete than calculations. Our measurements provide the atomic data needed for synthesizing accurate spectral models that cannot be provided with the same confidence using theoretical methods. In this sense, our EBIT facility and its spectroscopic equipment have become an analog computer where Nature computes the correct result for inclusion in

spectral codes.

Acknowledgments

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References

- A. J. Smith, P. Beiersdorfer, V. Decaux, K. Widmann, K. J. Reed, and M. H. Chen, Phys. Rev. A 54, 462 (1996).
- [2] G. Brown et al., Astrophys. J. **502**, 1015 (1998).
- [3] O. Bely and F. Bely, Sol. Phys. 2, 285 (1967).
- [4] R. Radtke, C. Biedermann, T. Fuchs, G. Fußmann, and P. Beiersdorfer, in preparation, 1999.
- [5] D. E. Post, R. V. Jensen, C. B. Tartar, W. H. Grasberger, and W. A. Lokke, At. Data Nucl. Data Tables 20, 397 (1977).
- [6] K. Fournier et al., in AIP Conference Proceedings 443, Atomic Processes in Plasmas 11th Topical Conference, edited by E. Oks and M. Pindzola, page 73, Woodbury, NY, 1998, AIP, AIP.
- [7] A. Smith et al., in preparation, 1999.
- [8] H. L. Zhang, D. H. Sampson, and R. E. H. Clark, Phys. Rev. A 41, 198 (1990).
- [9] A. Bar-Shalom, M. Klapisch, and J. Oreg, Phys. Rev. A 38, 1773 (1988).
- [10] G. Brown, P. Beiersdorfer, K. Reed, D. Liedahl, and K. Widmann, in preparation, 1999.
- [11] G.V. Brown et al., in preparation, 1999.
- [12] K. Berrington and J. Tully, Astron. Astrophys. Suppl. 126, 105 (1997).

[13] M. Gu et al., Astrophys. J. **518**, 1002 (1999).